

Determinants of high gas content and restoration of *in situ* gas content in Permian Wujiaping shale of the eastern Sichuan Basin, China

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Abstract The Permian Wujiaping Formation (P_3w) shale in eastern Sichuan Basin exhibits high gas content. Through total organic carbon (TOC) content determination, mineral composition analysis, N_2/CO_2 adsorption, high-pressure methane adsorption, and scanning electron microscopy experiments, we identified determinants of the high gas content and restored *in-situ* gas content. Findings demonstrate that the supercritical Dubinin–Astakhov (S-DA) model (based on micropore-filling theory) represents the optimal approach for accurately restoring the absolute adsorption amount of the third member of P_3w (P_3w^3) shale within the study region compared to the supercritical Langmuir (S-L) model (based on monolayer adsorption theory) widely used in the assessment of gas content of the Wufeng–Longmaxi shale. The P_3w^3 and Wufeng–Longmaxi shales have similar adsorption capacities at equivalent TOC levels, with the high adsorbed gas content of P_3w^3 attributed to the development of rich organic shale (with a TOC content of 7.68%) in

the anoxic reduction environment of the deep marine shelf facies. The high free gas content is due to the abundant siliceous minerals that play an anti-compaction and pore-preservation effect during the diagenesis, forming rich pore spaces (porosity of 6.05%). Under the influence of formation temperature and pressure, the *in-situ* gas content of P_3w^3 shale reservoir gradually increases with burial depth. The P_3w^3 shale gas reservoir with a burial depth of 4300–4400 m mainly exists in the free state, with the ratio of free gas to adsorbed gas approximately 7:3.

Keywords Wujiaping formation · Free gas · Adsorption model · *In-situ* gas content · Shale gas

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1 Introduction

Since the official commencement of shale gas exploration in 2009, China has dedicated over a decade to intensive technical research and large-scale development. These endeavors have led to remarkable breakthroughs in the Wufeng–Longmaxi shale gas fields within the Sichuan Basin. The cumulative proven reserves have surpassed $3 \times 10^{12} \text{ m}^3$, positioning China as a global benchmark for the commercial development of shale gas (Zhang et al. 2021; Guo et al. 2022; Bao et al. 2023; Jiang et al. 2023; Ma et al. 2023b; Zou et al. 2024). However, as the domestic energy consumption structure continues to be optimized and the “Carbon Peaking and Carbon Neutrality” initiatives are being vigorously advanced, the pressure for resource substitution in existing major production areas has become increasingly acute. Therefore, there is an urgent need to identify new exploration regions and target new geological formations. Such efforts are crucial to ensuring the stable and sustainable development of shale gas production, maintaining a reliable energy supply, and meeting broader carbon-neutrality objectives. By the end of 2022, Well DY1H in eastern Sichuan achieved a daily shale gas output of $32.06 \times 10^4 \text{ m}^3$ (Luo et al. 2025), which represents a significant breakthrough in the exploration of the P_3w shale gas in China, demonstrating the vast resource potential of P_3w shale gas. Field desorption tests indicate that the average gas content of P_3w^3 shale is $10.39 \text{ cm}^3/\text{g}$, substantially higher than that of the Wufeng–Longmaxi shale in the Pengshui area ($2.74 \text{ cm}^3/\text{g}$), Changning area ($2.87 \text{ cm}^3/\text{g}$), and Qianbei area ($3.78 \text{ cm}^3/\text{g}$) (Zhang 2019; Lu et al. 2022; Zhang et al. 2023a).

Shale gas, primarily methane (critical temperature: 190.4 K, critical pressure: 4.60 MPa) (Gasparik et al. 2012; Tang et al. 2017; Chang et al. 2024), exists in a supercritical state in reservoirs as: (1) adsorbed gas in organic/clay nanopores, (2) free gas in larger pores/microfractures, and (3) dissolved gas in formation water/residual oil (Ambrose et al. 2011; Gasparik et al. 2014; Hu et al. 2023). For over-mature shales with negligible liquid hydrocarbons, *in-situ* gas content can be considered as the sum of adsorbed gas and free gas (Zhang et al. 2023b). Current methodologies for quantifying free gas rely on the volumetric approach based on effective porosity and gas saturation (Feng et al. 2020). However, this method overestimates free gas content by double-counting adsorbed phase volume. To address this limitation, our study explicitly deducts adsorbed phase volume during calculation, resulting in more accurate free gas quantification. Laboratory methane adsorption tests ($<10 \text{ MPa}$) suggest that the adsorption amount increases with pressure (Wang et al. 2016). However, supercritical methane should exhibit declining adsorption amount above critical pressure (Feng et al. 2019). Thus, experimentally measured methane adsorption represents excess adsorption rather than absolute

adsorption. Through high-pressure methane adsorption experiments ($>30 \text{ MPa}$), the excess adsorption phenomenon was confirmed. Subsequently, the excess adsorption amount was converted into absolute adsorption amount by adsorption model to characterize the adsorption capacity of the P_3w shale.

The most widely used absolute adsorption amount correction model at present is the supercritical Langmuir (S-L) model, which is based on the monolayer adsorption theory. This model has achieved remarkable results in the assessment of adsorption capacity in the Wufeng–Longmaxi shale (Feng et al. 2020; Chen et al. 2021; Zhou and Zhang 2023). However, in this paper, the S-L model was compared with the supercritical Dubinin–Radushkevich (S-DR) and supercritical Dubinin–Astakhov (S-DA) models based on the micropore-filling theory for the P_3w shale (Wang et al. 2023a, b, c; Li et al. 2024). The results showed that the S-DA model had the best correction effect. The adsorption mechanism study indicated that the P_3w shale simultaneously possesses both micropore-filling and monolayer adsorption mechanisms. Therefore, the S-DA model was ultimately selected for estimating the *in-situ* gas content of P_3w shale.

Although the P_3w^3 shale in the eastern Sichuan exhibits remarkable characteristics of high gas content, there are still gaps in the understanding of its determinants and the distribution of the *in-situ* gas content in the reservoir. These gaps have restricted the development of shale gas exploration and development in this area. This study establishes that deep-water shelf facies sedimentation under anoxic reducing conditions controls development of highly mature, organic-rich shale, constituting the primary mechanism for high adsorbed gas content of the P_3w^3 shale. Concurrently, abundant siliceous minerals mitigate porosity reduction during diagenesis, while pyrite intercrystalline pores provide essential reservoir space for free gas. These dual controls synergistically drive high-gas-content of the P_3w^3 shale, establishing the scientific basis for gas occurrence studies and “Geological sweet spots” prediction in the eastern Sichuan Basin (Wang et al. 2023a, b; Zhang et al. 2023c).

2 Geological setting

The Sichuan Basin, one of the four major basins in western China, lies on the western margin of the Yangtze Plate. In light of its regional tectonic features, the basin has been partitioned into six second-order tectonic units. The study area is situated within the middle-uplift and steep-faulted fold belt in the eastern part of the Sichuan Basin. (Fig. 1A; Jiao et al. 2021; Ma et al. 2023a). During the Permian period, the eastern Sichuan Basin was characterized by marine sedimentation. Successively, shoreline–tidal flat facies, carbonate platform facies, slope facies, and deep-water shelf facies

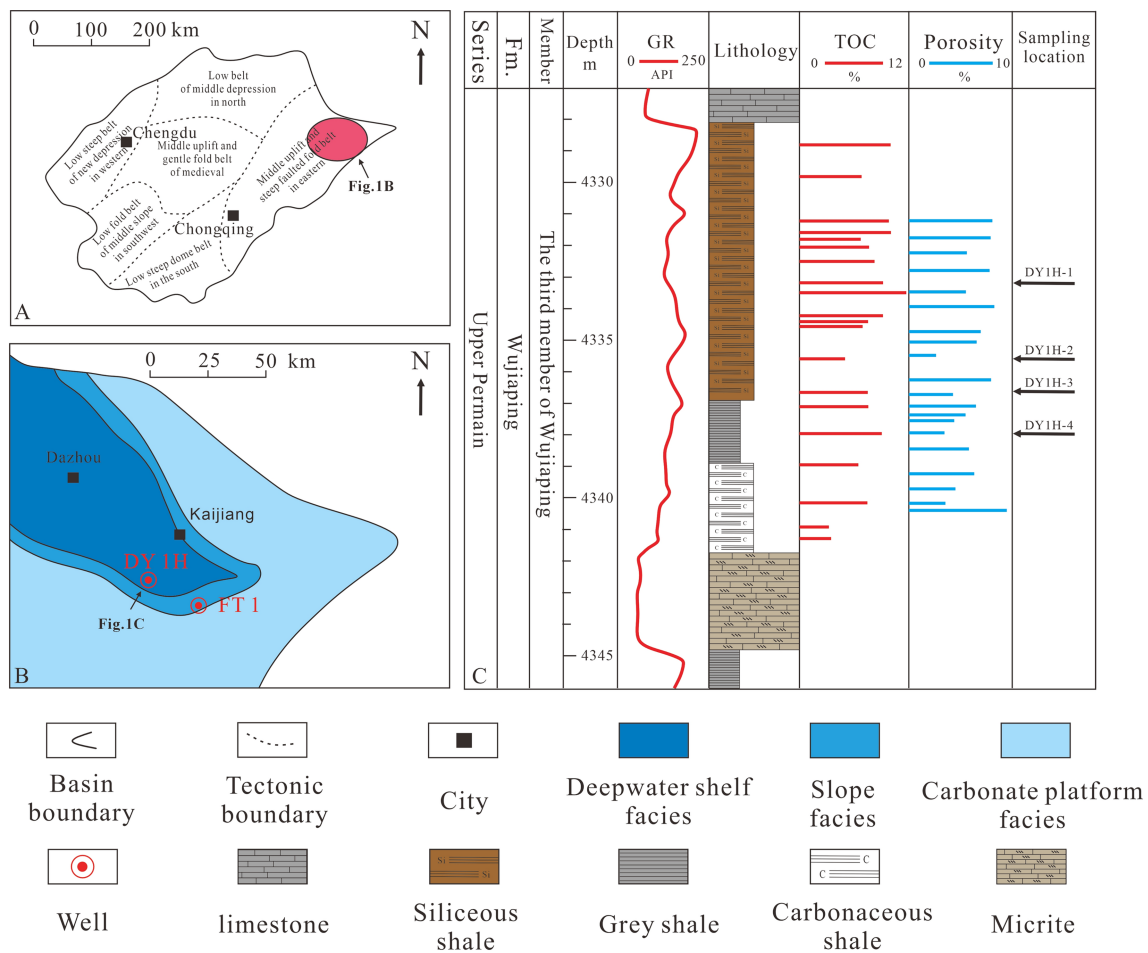


Fig. 1 Regional geological survey map of the study area and sample well column map of P_3w^3 : **A** second-order tectonic units map of Sichuan Basin; **B** plane diagram of P_3w^3 sedimentary period in the study area; **C** column diagram of P_3w^3 in Well DY1H

were deposited (Fig. 1B; Qiu et al. 2024; Yi et al. 2024). This depositional evolution led to the formation of P_3w , which consists predominantly of limestone and siliceous shale. P_3w^3 , the target stratum of this study, was deposited in the deep-water shelf. It is primarily composed of black siliceous shale and mixed shale interbedded with calcareous shale, argillaceous limestone, and carbonaceous shale (Fig. 1C). The organic matter in P_3w^3 shale belongs to the Type II₁–II₂ and has reached an over-mature stage of thermal evolution, with a vitrinite reflectance (R_o) greater than 2.0%.

3 Samples and experimental methods

The experimental samples are P_3w^3 black shale in eastern Sichuan, from Well DY1H and Well FT1 deployed by Southwest Oil and Gas Company, along with outcrop profiles at XBX. Total organic carbon (TOC) content, mineral composition analysis by X-ray diffraction (XRD), gas (CO_2 and N_2) adsorption, and high-pressure methane adsorption

(HPMA) tests at 363.15 K were carried out on the well samples. HPMA tests at 323.15 K, 343.15 K, and 393.15 K were also carried out for the DY1H-2 and DY1H-3 samples. The outcrop samples were observed by field-emission scanning electron microscopy (FE-SEM).

3.1 TOC content and mineral composition

Procedures followed GB/T 19145-2022. First, 5.00 g of pulverized sample (<150 μ m) was acid-treated with 3 mol/L HCl at 343.15 K for 24 h to remove inorganic carbon. Then, the residues were washed to neutrality and dried under N_2 . Finally, TOC was quantified using a multi N/C 3100 analyzer via combustion at 1223.15 K in pure O_2 , with CO_2 measured by a non-dispersive infrared detector.

All the procedures adhered to Standard SY/T 5163-2018. Initially, 0.2 g of pulverized sample (<40 μ m) was dried at 333.15 K for 4 h to remove hygroscopic moisture. Subsequently, XRD analysis was performed using a Bruker D8 DISCOVER instrument. Finally, quantitative

phase analysis was conducted using the K-value method, calibrated against National Institute of Standards & Technology (NIST) Standard Reference Material 1976 corundum ($\alpha\text{-Al}_2\text{O}_3$) standard.

3.2 CO_2 and N_2 adsorption

All the procedures adhered to Standard GB/T 21650-2011 and ISO 15901-2022. Measurements were performed using a Specific Surface Area and Porosity Analyzer (ASAP 2460), and 8.00 g of pulverized sample ($<180\ \mu\text{m}$) was degassed under vacuum at 383.15 K for 10 h, ensuring complete removal of physisorbed contaminants while preserving structural integrity.

CO_2 adsorption/desorption analysis was conducted at 273.15 K with relative pressure (P/P_0) ranging from 0.001 to 0.998. Micropore volume and specific surface area were calculated using density functional theory.

N_2 adsorption/desorption isotherms were measured at 77.35 K over $P/P_0 = 0.001\text{--}0.998$. The mesopore volume distribution was derived from the desorption branch using the Barrett–Joyner–Halenda model, while the specific surface area was determined via the Brunauer–Emmett–Teller model within the validated P/P_0 range (0.05–0.30).

3.3 HPMA

High-pressure methane adsorption isotherms (0.1–35 MPa) were measured gravimetrically in compliance with Standard GB/T 35210.2-2020, using a magnetic levitation balance (ISOSORP-HP; resolution: 0.01 mg). First, 10 g of pulverized sample ($<100\ \mu\text{m}$) was degassed at 383.15 K for 12 h. Then, a buoyancy test was conducted using He as the medium, and the adsorbed mass was recorded at 15 pressure points upon reaching equilibrium (mass drift $<5\ \mu\text{g}/\text{min}$ for 2 h). Finally, volumetric adsorption amount (cm^3/g) was derived from mass changes via molar volume normalization with a buoyancy correction.

3.4 FE-SEM

Samples were cut into $3\ \text{mm} \times 3\ \text{mm} \times 1\ \text{mm}$ pieces and polished with argon ions. After that, they were cleaned with absolute ethanol and dried under vacuum at 333.15 K. A thin layer of carbon was sputtered onto the polished surface to enhance conductivity. The prepared sample was then placed in a Quanta 650 FEG FE-SEM from FEI. With an acceleration voltage of 10–15 kV and a beam-spot size of 3.0–3.5, pores were observed using a combination of secondary and backscattered electron probes.

4 Results

4.1 Geochemical and mineralogical characteristics

The TOC content in the P_3w^3 shale of Well DY1H ranged from 5.03% to 10.00% (average: 7.68%), while that of Well FT1 ranged from 1.12% to 11.40% (average: 5.02%). The main inorganic minerals in the P_3w^3 shale were siliceous, clay, and carbonate minerals, accounting for 14.33%–89.36% (average: 44.52%), 0%–59.61% (average: 17.14%), and 2.34%–81.30% (average: 27.46%), respectively (Table 1). Other mineral components mainly included pyrite and feldspar.

4.2 High-pressure methane adsorption characteristics

4.2.1 Results of HPMA experiment

As the pressure increased, the shale samples exhibited a consistent trend in measured methane adsorption amount (n_{msd}) (Fig. 2A, C, D). During the low-pressure stage, n_{msd} rose steeply with increasing pressure. As the pressure continued to increase, the growth of n_{msd} slowed, reaching its maximum value at 12 MPa. When the pressure exceeded 12 MPa, n_{msd} declined with varying amplitudes, which occurs because the density difference between adsorbed and free methane under supercritical conditions changes with increasing pressure. At low pressures, the adsorbed methane density substantially exceeds that of free methane. As the pressure rises, however, some methane in the adsorption space approaches free methane density. This portion, termed “quasi-adsorbed methane” ($\rho_g \times V_a$), represents methane poised to transition from the adsorption space to the free space (Fig. 3; Feng 2020; Chang et al. 2024). Since quasi-adsorbed methane and free methane exhibit identical densities, they cannot be distinguished by HPMA experiments. Consequently, a decrease in n_{msd} occurs with increasing pressure during the high-pressure stage.

4.2.2 Excess adsorption model of methane

Gibbs et al. (Gibbs 1878; Curtis 2002; Sakurovs et al. 2008; Gensterblum et al. 2013) have proposed that “excess adsorption amount” (n_{ex}) represents n_{msd} , while the actual adsorption amount, also known as the absolute adsorption amount (n_{abs}), should be the sum of n_{ex} and the quasi-adsorption amount (Eq. 1), and the relationship between n_{abs} and n_{ex} is thus established (Eqs. 2, 3):

$$n_{\text{abs}} = n_{\text{ex}} + \rho_g \times V_a \quad (1)$$

$$V_a = \frac{n_{\text{abs}}}{\rho_a} \quad (2)$$

Table 1 TOC and mineral composition of samples

Sample ID	Depth, m	TOC, %	Siliceous minerals, %	Clay minerals, %	Carbonate minerals, %
DY1H-1	4333.12	9.18	27.28	47.00	25.72
DY1H-2	4335.66	5.03	58.90	11.39	25.36
DY1H-3	4336.70	7.47	55.60	18.30	20.50
DY1H-4	4337.98	9.03	56.52	28.50	14.98
DY1H-5	4328.85	10.00	20.10	52.03	2.34
DY1H-6	4329.87	6.81	21.82	59.61	1.23
DY1H-7	4332.05	7.63	25.51	17.51	37.91
DY1H-8	4332.55	8.22	45.73	9.30	20.04
DY1H-9	4334.62	6.94	72.11	6.61	6.81
DY1H-10	4338.97	6.45	40.33	4.73	44.52
FT1-1	4558.32	7.20	48.65	5.00	36.96
FT1-2	4559.49	3.11	39.57	0.00	54.35
FT1-3	4560.5	2.21	14.33	0.00	81.30
FT1-4	4575.76	1.12	24.26	8.03	57.10
FT1-5	4576.26	4.32	89.36	3.22	4.93
FT1-6	4576.53	4.27	33.90	23.57	23.19
FT1-7	4578.03	6.49	69.79	4.78	18.41
FT1-8	4592.62	11.40	57.59	8.85	18.55

$$n_{\text{ex}} = n_{\text{abs}} \times \left(1 - \frac{\rho_g}{\rho_a}\right) \quad (3)$$

where n_{abs} (cm^3/g) is the absolute adsorption amount, n_{ex} (cm^3/g) is the excess adsorption amount, ρ_g (g/cm^3) is the density of free methane, V_a (cm^3) is the volume of the adsorption space, and ρ_a (g/cm^3) is the density of adsorbed methane.

Numerous models have been put forward to elucidate methane adsorption on shale. By integrating these models with Eq. (3), a model tailored for supercritical methane adsorption was developed.

4.2.2.1 Supercritical Langmuir (S-L) model Drawing on Langmuir theory, previous studies have posited that kerosene captures methane and arranges it in a monolayer on its surface (Langmuir 1918; Krooss et al. 2002; Gasparik et al. 2012), and the S-L model is expressed as:

$$n_{\text{ex}} = \frac{V_L \times P}{P + P_L} \times \left(1 - \frac{\rho_g}{\rho_a}\right) \quad (4)$$

where V_L (cm^3/g) is the Langmuir volume, representing the theoretical maximum adsorption amount and the strength of shale adsorption capacity, P_L (MPa) is the Langmuir pressure, which is the pressure corresponding to half of V_L (MPa) which is the experimental pressure.

4.2.2.2 Supercritical Dubinin–Radushkevich (S-DR) model Based on Polanyi's adsorption potential theory,

methane fills micropores sequentially in accordance with the magnitude of adsorption potential (Dubinin 1960, 1989; Amankwah et al. 1995; Krooss et al. 2002), and the S-DR model is expressed as:

$$n_{\text{ex}} = V_0 \exp \left\{ -D \left[\ln \left(\frac{\rho_a}{\rho_g} \right) \right]^2 \right\} \times \left(1 - \frac{\rho_g}{\rho_a}\right) \quad (5)$$

where V_0 (cm^3/g) is the maximum adsorption amount and representing the strength of shale adsorption capacity, and D is the characteristic parameter, dimensionless.

4.2.2.3 Supercritical Dubinin–Astakhov (S-DA) model During investigations of the S-DR model, some scholars discovered that replacing the fixed parameter 2 with an undetermined parameter (k) enhanced the model's applicability (Xiong et al. 2015; Zhou et al. 2017a), and the S-DA model is expressed as:

$$n_{\text{ex}} = V_0 \exp \left\{ -D \left[\ln \left(\frac{\rho_a}{\rho_g} \right) \right]^k \right\} \times \left(1 - \frac{\rho_g}{\rho_a}\right) \quad (6)$$

4.2.3 Model validation and restoration of n_{abs}

According to previous studies, parameters such as the density of adsorbed methane (ρ_a) are regarded as undetermined parameters to obtain the most accurate results through mathematical optimization fitting (Rexer et al.

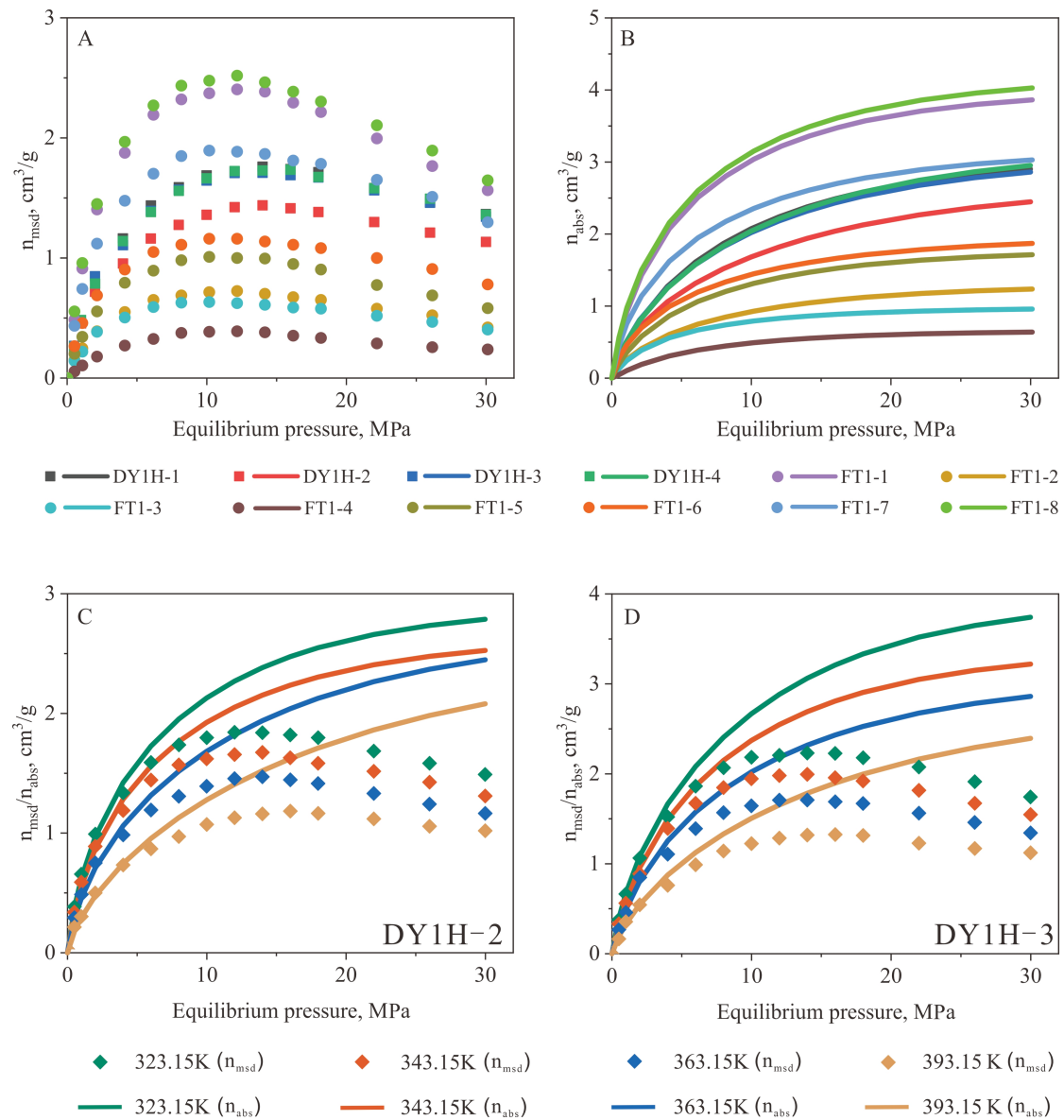


Fig. 2 HPA experiment results and n_{abs} restored by the S-DA model: **A** n_{msd} of different samples at 363.15 K; **B** n_{abs} of different samples at 363.15 K; **C** n_{msd} and n_{abs} of DY1H-2 at different temperatures; and **D** n_{msd} and n_{abs} of DY1H-3 at different temperatures

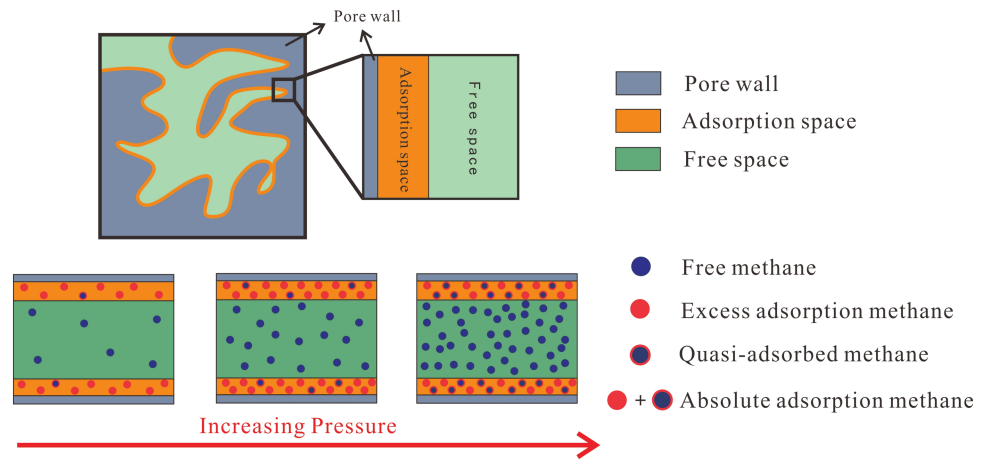
2013; Tian et al. 2016; Feng 2020). The density of free methane (ρ_g) under different temperatures and pressures can be obtained by querying the NIST database, and the parameter values obtained by fitting different models are slightly different (Tables 2, 3, 4).

The fitting correlation coefficient (R^2) serves as an indicator of the goodness-of-fit. A larger R^2 value corresponds to a better fitting effect. The root mean square error (RMSE) quantifies the deviation between the fitted values and the measured values. A smaller RMSE value implies that the fit is more in line with the actual situation (Eq. 7).

$$\text{RMSE} = \sqrt{\frac{1}{N} \times \sum_{i=1}^N (n_{\text{msd}} - n_{\text{fit}})^2} \quad (7)$$

where N is the number of data points used for fitting, and n_{fit} is the excess adsorption amount fitted by the model.

The R^2 values of the three models exceed 0.99, demonstrating excellent fitting performance. Among them, the S-DA model shows a slightly higher R^2 than the S-DR and S-L models. The RMSE values of all three models are less than 0.05, indicating minimal fitting errors and high fitting

Fig. 3 Pore space microscopic interpretation (modified from Tang et al. 2017)**Table 2** S-L model fitting parameters at 363.15 K

Sample	V_L , cm ³ /g	ρ_a , g/cm ³	P_L , MPa
DY1H-1	3.51	0.307	6.93
DY1H-2	2.44	0.356	5.01
DY1H-3	3.23	0.325	6.15
DY1H-4	3.35	0.322	6.59
FT1-1	4.26	0.279	4.22
FT1-2	1.39	0.255	5.15
FT1-3	1.10	0.277	3.94
FT1-4	0.87	0.235	7.57
FT1-5	1.98	0.246	5.21
FT1-6	1.94	0.305	3.74
FT1-7	3.16	0.311	3.74
FT1-8	4.34	0.288	4.04

Table 4 S-DA model fitting parameters at 363.15 K

Sample	V_0 , cm ³ /g	ρ_a , g/cm ³	D	k
DY1H-1	3.12	0.300	0.166	1.75
DY1H-2	2.74	0.295	0.231	1.47
DY1H-3	3.12	0.301	0.184	1.66
DY1H-4	3.24	0.296	0.205	1.60
FT1-1	4.01	0.270	0.124	1.84
FT1-2	1.29	0.247	0.172	1.69
FT1-3	0.98	0.280	0.080	2.10
FT1-4	0.66	0.246	0.138	1.96
FT1-5	1.77	0.242	0.156	1.76
FT1-6	1.96	0.280	0.137	1.74
FT1-7	3.18	0.286	0.130	1.76
FT1-8	4.20	0.273	0.128	1.80

Table 3 S-DR model fitting parameters at 363.15 K

Sample	V_0 , cm ³ /g	ρ_a , g/cm ³	D
DY1H-1	2.86	0.324	0.109
DY1H-2	2.22	0.357	0.092
DY1H-3	2.74	0.337	0.103
DY1H-4	2.78	0.339	0.105
FT1-1	3.83	0.280	0.096
FT1-2	1.17	0.263	0.106
FT1-3	1.01	0.274	0.095
FT1-4	0.65	0.248	0.129
FT1-5	1.65	0.253	0.108
FT1-6	1.81	0.299	0.088
FT1-7	2.96	0.304	0.088
FT1-8	3.96	0.286	0.093

accuracy, with the S-DA model generally having a slightly smaller RMSE (Fig. 4A, B). The ρ_a values obtained from the three models fall between the critical methane density

(0.162 g/cm³) and the methane density of boiling liquid at atmospheric pressure (0.424 g/cm³) (Harpalani et al. 2006; Gasparik et al. 2012; Wang et al. 2016), validating the reasonableness of the fitting results (Fig. 4C). In conclusion, compared with the S-L and S-DR models, the S-DA model is more suitable for restoring the n_{ex} of shale in the study area to n_{abs} (Fig. 2B–D).

5 Discussion

5.1 Adsorption mechanism of supercritical methane

Hypothesis 1 In P_3w^3 shale, supercritical methane is adsorbed on the pore walls of meso-/macropores in a monolayer arrangement only. The volume of the adsorption space (V_{a-SL}) (Eq. 8) and the average kinetic diameter of the methane molecules (σ) (Eq. 9) are calculated. Then, combined with the specific surface area of meso-/macropore specific

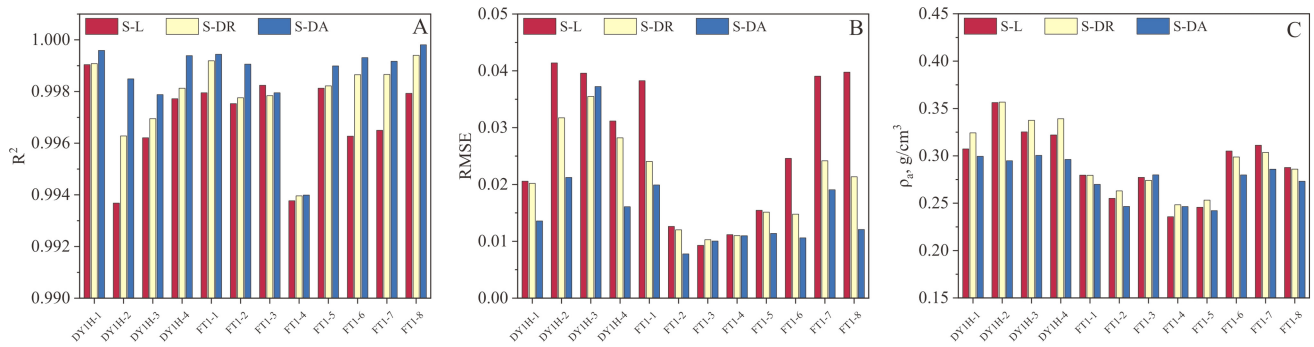


Fig. 4 Model applicability analysis

surface area ($S_{\text{mes-mac}}$), the number of adsorbed molecular layers (λ) of methane on the meso-/macropores is computed (Eq. 10; Table 5):

$$V_{\text{a-SL}} = \frac{V_L \times M}{V_M \times \rho_{\text{a-SL}}} \quad (8)$$

$$\sigma = \left(\frac{M}{N_A \times \rho_a} \right)^{\frac{1}{3}} \quad (9)$$

$$\lambda = \frac{V_{\text{a-SL}}}{S_{\text{mes-mac}} \times \sigma} \quad (10)$$

where $V_{\text{a-SL}}$ (cm^3/g) is the calculated adsorption space volume, M is the molar mass of methane, with a value of 16 g/mol, V_m is the molar volume of gas under standard conditions, with a value of 22.4 L/mol, $\rho_{\text{a-SL}}$ (g/cm^3) is the adsorbed methane density fitted by the S-L model, σ (nm) is the average kinetic size of methane molecules, N_A is Avogadro's constant, with a value of $6.02 \times 10^{23} \text{ mol}^{-1}$, λ is the number of adsorbed methane molecular layers, and $S_{\text{mes-mac}}$

(m^2/g) is the specific surface area of the meso-/macropores calculated by the gas adsorption experiment.

Hypothesis 2 For supercritical methane adsorption in P_3w^3 shale, there exists only a micropore-filling adsorption mechanism. The adsorption space volume is calculated based on the maximum adsorption amount ($V_{0\text{-DR}}$ and $V_{0\text{-DA}}$) and ρ_a fitted by the S-DR and S-DA models (Eqs. 11, 12; Table 5):

$$V_{\text{a-SDR}} = \frac{V_{0\text{-SDR}} \times M}{V_M \times \rho_{\text{a-SDR}}} \quad (11)$$

$$V_{\text{a-SDA}} = \frac{V_{0\text{-SDA}} \times M}{V_M \times \rho_{\text{a-SDA}}} \quad (12)$$

where $V_{\text{a-SDR}}$ (cm^3/g) and $V_{\text{a-SDA}}$ (cm^3/g) are the calculated adsorption space volumes, $V_{0\text{-SDR}}$ (cm^3/g) and $V_{0\text{-SDA}}$ (cm^3/g) are the fitted maximum adsorption amounts, respectively, and $\rho_{\text{a-SDR}}$ (g/cm^3) and $\rho_{\text{a-SDA}}$ (g/cm^3) are the adsorbed methane densities fitted by S-DR and S-DA model, respectively.

Table 5 Adsorption mechanism parameters

Sample ID	$V_{\text{a-SL}}$, cm^3/g	σ , nm	$S_{\text{mes-mac}}$, cm^2/g	λ	$V_{\text{a-SDR}}$, cm^3/g	$V_{\text{a-SDA}}$, cm^3/g	V_{mic} , cm^3/g
DY1H-1	0.0082	0.442	4.52	4.1	0.0063	0.0074	0.0035
DY1H-2	0.0049	0.421	3.08	3.8	0.0044	0.0066	0.0031
DY1H-3	0.0071	0.434	4.49	3.6	0.0058	0.0074	0.0033
DY1H-4	0.0074	0.435	7.18	2.4	0.0059	0.0078	0.0043
FT1-1	0.0108	0.456	5.25	4.5	0.0098	0.0106	0.0034
FT1-2	0.0039	0.470	2.04	4.1	0.0032	0.0037	0.0013
FT1-3	0.0028	0.458	1.43	4.3	0.0026	0.0025	0.0009
FT1-4	0.0026	0.483	0.67	8.1	0.0019	0.0019	0.0005
FT1-5	0.0058	0.476	2.50	4.8	0.0046	0.0052	0.0019
FT1-6	0.0045	0.443	1.63	6.3	0.0043	0.0050	0.0011
FT1-7	0.0072	0.440	3.23	5.1	0.0070	0.0079	0.0021
FT1-8	0.0108	0.452	7.83	3.1	0.0099	0.0110	0.0049

The λ values obtained under Hypothesis 1 range from 2.4 to 8.1, all of which are greater than 1 (Table 5), which contradicts the monolayer adsorption theory. Thus, the supercritical methane adsorption in P_3w^3 shale does not solely follow the monolayer adsorption mechanism. The V_{a-SDR} and V_{a-SDA} values obtained under Hypothesis 2 are both larger than the micropore volume (V_{mic}) determined from gas adsorption experiments (Table 5). If adsorption occurs entirely according to the micropore-filling theory, V_{a-SDR} and V_{a-SDA} should be less than or equal to V_{mic} . Therefore, the supercritical methane adsorption in P_3w^3 shale does not completely rely on the micropore-filling mechanism. Based on the above analysis, it is hypothesized that both micropore-filling and monolayer adsorption mechanisms co-exist for supercritical methane in P_3w^3 shale. Given that the adsorption potential of micropores is higher than that of meso-/macropores, at low pressures, methane first enters the micropores with higher adsorption potential (Sheng et al. 2014; Liu et al. 2016; Zhou et al. 2017b). Monolayer adsorption then forms on the surface of meso-/macropores when micropore filling is nearly saturated.

5.2 Determinants of high gas content

The differential enrichment mechanisms of adsorbed versus free gas in shale reservoirs are governed by distinct geological controls. The proportion of adsorbed gas varies significantly, typically accounting for 20%–85% of total gas in North American shale plays and 30%–50% in South China's commercially viable reservoirs (Curtis 2002; Wang et al. 2015; Zou et al. 2017). Elevated adsorbed gas content fundamentally depends on organic matter (OM) abundance, which provides both hydrocarbon-generating macerals and nanoscale OM pore networks that dominate methane adsorption. Conversely, free gas content is directly governed by

porosity. The specific calculation can be found in Sect. 5.3.1, which enables essential bulk-phase storage capacity within the shale reservoirs.

5.2.1 High adsorbed gas content

Through a correlation analysis of TOC content and inorganic mineral components with the shale adsorption capacity (V_0), it was found that OM is the primary component controlling the adsorption capacity of P_3w^3 shale (Fig. 5). Specifically, the higher the TOC content, the greater the V_0 . FE-SEM observations revealed that the OM in P_3w^3 shale exhibited irregularly elongated or massive morphologies, with well-developed OM pores (Fig. 6A–C). These pores are mainly spherical and honeycombed in shape (Fig. 6C). The development of OM pores provides storage space for the existence of adsorbed gas (Zhang et al. 2024).

The OM in the Wufeng–Longmaxi shale is also in the over-mature stage, with $R_o > 2.0\%$, but, unlike the P_3w^3 shale, it mainly comprises the Type I–II₁. Through a comparison of the TOC– V_0 correlation analysis for the Wufeng–Longmaxi shale, it was found that the OM in these two sets of shales controls the shale adsorption capacity to a similar extent (Fig. 5A), which demonstrates that, for over-mature OM, the shale adsorption capacity is governed by the TOC content rather than by the OM type. In Well DY1H, the average TOC content of P_3w^3 shale is 7.68%, corresponding to the V_0 of 3.72 cm³/g., which is higher than the 2.45% TOC content of the Wufeng–Longmaxi shale (corresponding to the V_0 of 1.96 cm³/g) (Zhang 2019; Wang 2020, 2023c) and approaches or surpasses TOC values of typical U.S. commercial gas-bearing shales (Table 6). Thus, a high TOC content is the main controlling factor for the formation of high adsorbed gas content in P_3w^3 shale.

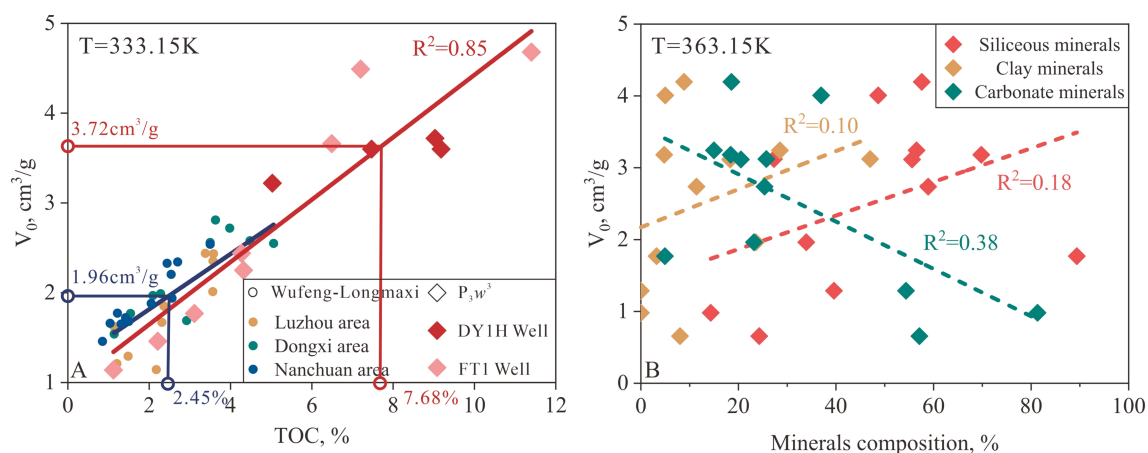


Fig. 5 Control factors of V_0 in P_3w^3 shale and control of TOC content on V_0 in the Wufeng–Longmaxi shale (data source: Zhang 2019; Wang 2020, 2023c)

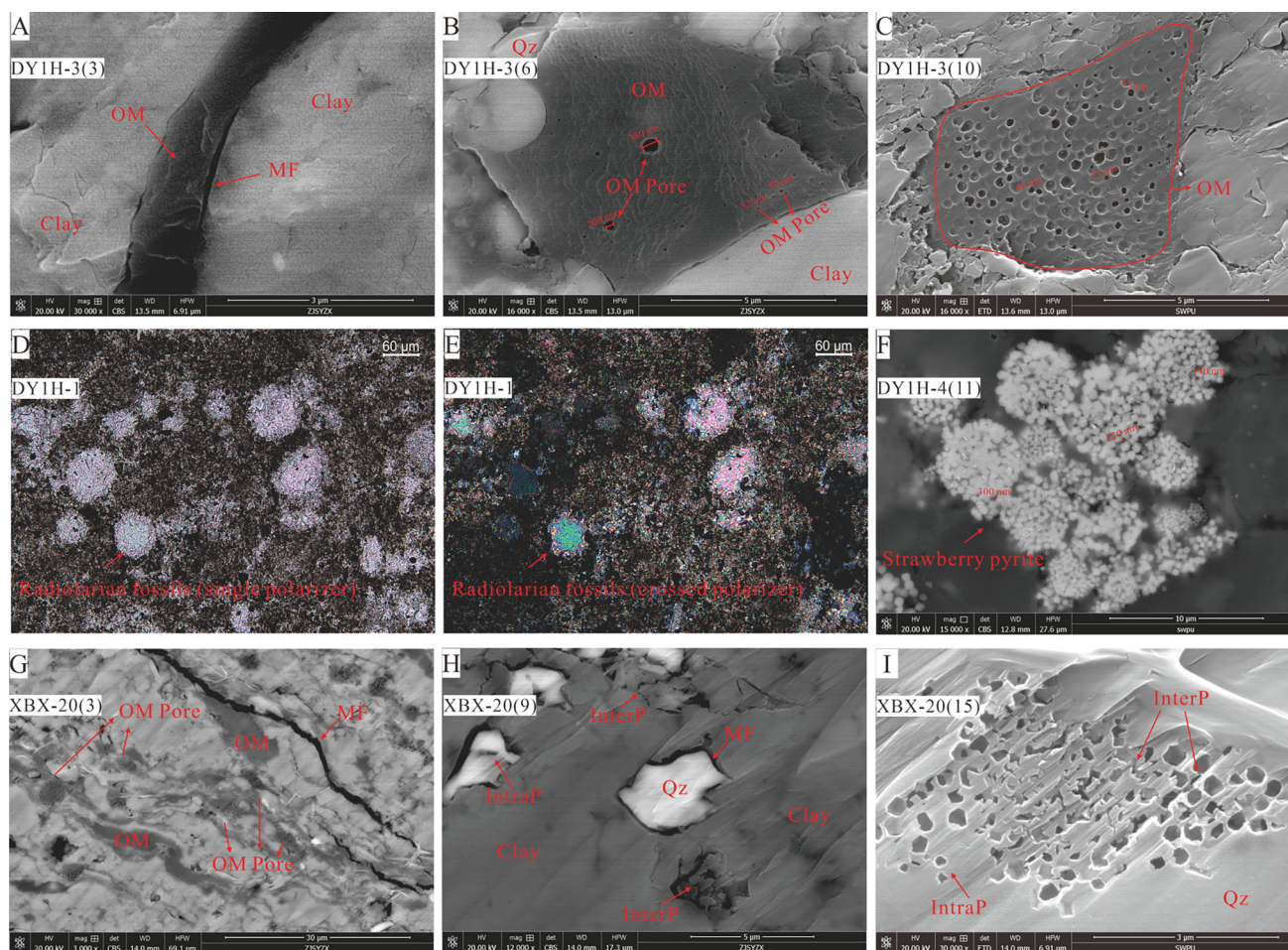


Fig. 6 SEM (A–C, F and G–I) and thin section (D and E) analysis of P_3w^3 shale; 3, 6, and 10 respectively represent the 3rd, 6th and 10th fields of view when observing the sample

Table 6 Comparative analysis of marine shale characteristics: Wujiaping formation (eastern Sichuan Basin) versus global productive formations (data source: Curtis 2002; Zhang 2019; Wang 2020, 2023c)

Characteristic	Shale					
	Wujiaping	Wufeng–Longmaxi	Barnett	Ohio	Antrim	New Albany
Region	Eastern Sichuan Basin	Southeastern Sichuan Basin	Texas	Kentucky	Michigan	Indiana
System	Permian	Ordovician–Silurian	Mississippian	Devonian	Devonian	Devonian
Depth/m	4000–5000	1500–4500	1981–2591	610–1524	183–732	183–1494
Effective thickness/m	20–50	84–102	15–61	9–30	21–37	15–30
Kerogen type	II ₂ –II ₁	II ₁ –I	II	II–I	I	II
R _o /%	2.5–3.0	1.6–3.6	1.0–1.3	0.4–1.3	0.4–0.6	0.4–1.0
TOC/%	<u>5.03–9.18</u> 7.68	<u>0.85–5.06</u> 2.45	4.5	0–4.7	0.3–24.0	1.0–25.0
Porosity/%	<u>2.61–9.47</u> 6.05	<u>0.7–5.48</u> 2.83	4.0–5.0	4.7	9.0	10.0–14.0
Gas content /(cm ³ /g)	<u>7.36–16.16</u> 10.39	<u>1.59–8.68</u> 3.13	8.50–9.91	1.70–2.83	1.13–2.83	1.13–2.27

Note: The numbers above the underline represent the ranges of TOC, porosity and gas content, while the numbers below the underline represent the average values of the former

The high TOC content is primarily controlled by the sedimentary environment. The deep-water shelf setting, characterized by persistent anoxia and reducing conditions, enables enhanced preservation of planktonic and algal biomass after death (Fig. 6D, E), providing substantial organic material which becomes the source for subsequent shale hydrocarbon generation (Luo et al. 2025). With R_o greater than 2.0%, the P_3w^3 shale resides in the over-mature stage. This combination of elevated organic richness and advanced thermal maturity drives extensive organic pore development, facilitating adsorbed gas storage.

5.2.2 High free gas content

In P_3w^3 shale, inorganic minerals exhibit several pore types. Intraparticle pores are mainly found within rigid mineral particles like quartz, presenting an isolated form. Interparticle pores are typically in the shape of irregular polygons, formed at the contact points of particle accumulations, with locally developed large pores. Microfractures are distributed in a narrow and elongated manner (Fig. 6G–I), and, in contrast to adsorbed gas in small-sized organic pores, free gas has a tendency to reside in inorganic pores and microfractures with relatively larger pore sizes (Ma et al. 2024; Cheng et al. 2025).

The porosity of P_3w^3 shale ranges from 2.61% to 9.47% (average: 6.05%), significantly exceeding values from the Wufeng–Longmaxi shale in the Dongxi area (1.94%–3.95%, average 3.00%), Changning area (1.72%–5.48%, average 3.68%), Chuannan area (0.7%–2.09%, average 1.44%), and Qianbei area (1.36%–3.86%, average: 3.02%) (Fig. 7A; Luo 2019; Xiao 2022; Yang 2022; Wang 2023b), and approaching or surpassing typical U.S. commercial gas-bearing shales porosities (Table 6). The *in-situ* free gas estimation equations (Eqs. 17, 18) indicate that the free gas amount under constant burial conditions (temperature and pressure

variations are minimal) increases as porosity rises. Thus, the high porosity of P_3w^3 shale serves as the foundation for the formation of high free gas content.

The siliceous mineral content in P_3w^3 shale exhibits a positive correlation with porosity (Fig. 7B), demonstrating that siliceous mineral's resistance to compaction and pore preservation during diagenesis governs high reservoir porosity. Concurrently, anoxic-reducing conditions facilitate the development of strawberry pyrite (Fig. 6F), whose crystalline frameworks generate intercrystalline pores that host free gas accumulation.

5.3 Restoration of *in-situ* gas content

5.3.1 Estimation model

Given that the solubility of methane in water is extremely low and that the OM in the over-mature stage typically exists as solid asphalt with no liquid hydrocarbons present, only adsorbed gas and free gas are taken into account when restoring the *in-situ* gas content of the reservoir (Curtis 2002; Montgomery et al. 2005). From the research in 4.2.3, the S-DA model is deemed the most suitable for restoring n_{abs} in P_3w^3 shale. Thus, the S-DA model is also employed for estimating the *in-situ* adsorbed gas content. The key to accurate prediction lies in understanding how the S-DA model parameters (V_0 , D , k and ρ_a) vary under reservoir conditions. Since these parameters are derived from fitting HPMA experimental (0–30 MPa) data at constant temperatures, reflecting inherent adsorbent properties or adsorbent–adsorbate interaction strengths at constant temperatures, the pressure changes do not substantially alter these intrinsic characteristics (Feng et al. 2020; Chen et al. 2021). Crucially, however, these properties exhibit significant variations across different

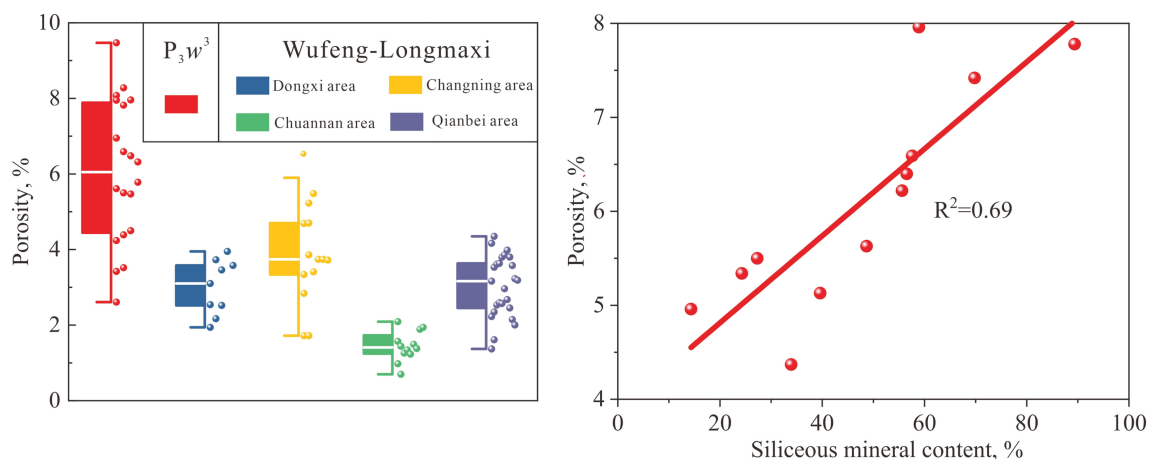


Fig. 7 Porosity comparison: (A) P_3w^3 versus Wufeng–Longmaxi shale; (B) siliceous mineral content and porosity correlation of P_3w^3 shale

Table 7 S-DA model fitting parameters of samples DY1H-1 and DY1H-2 at different temperatures

Sample; T, K	Parameters				
	V_0 , cm ³ /g	ρ_a , g/cm ³	D	k	
DY1H-2	323.15	2.99	0.395	0.120	1.80
	343.15	2.70	0.351	0.122	1.81
	363.15	2.73	0.295	0.231	1.47
	393.15	2.50	0.270	0.338	1.33
DY1H-3	323.15	4.08	0.356	0.183	1.63
	343.15	3.44	0.332	0.144	1.80
	363.15	3.12	0.301	0.184	1.66
	393.15	2.78	0.266	0.301	1.42

temperatures (Table 7), meaning that parameters for the same sample differ substantially at distinct thermal conditions. Therefore, establishing relationships between these parameters and temperature variations becomes essential, Eqs. (13–16) present the variation of DY1H-3 sample parameters with temperature:

$$V_0 = -0.018 \times T + 9.730 \quad (13)$$

$$D = 1.83 \times 10^{-3} \times T - 0.451 \quad (14)$$

$$k = 3.67 \times 10^{-3} \times T + 2.927 \quad (15)$$

$$\rho_a = -1.31 \times 10^{-3} \times T + 0.777 \quad (16)$$

In traditional research, the entire effective reservoir space of a reservoir was utilized to estimate the free gas amount (n_f^{con}) (Eq. 17), which led to an overestimation of the free gas reservoir space (Lewis et al. 2004; Ambrose et al. 2011). In this study, to guarantee the accuracy of free gas content estimation, the actual free gas amount (n_f) (Eq. 18) was derived by subtracting the adsorption space volume (Eqs. 2, 6) from the effective storage space volume calculated using the traditional method. The gas in place (GIP) can be expressed as the sum of n_{abs} and n_f , and, numerically, it is also equivalent to the sum of n_{ex} and n_f^{con} (Eq. 19). Notably, since dry samples were used in this experiment and actual formation moisture would reduce shale adsorption capacity; Eq. (19) and discussion in Sect. 5.3.2 represent the theoretical maximum *in-situ* gas content:

$$n_f^{\text{con}} = \frac{\varphi \times (1 - S_w - S_o) \times \rho_g \times C_{\text{STP}}}{\rho_{\text{bulk}}} \quad (17)$$

$$n_f = n_f^{\text{con}} - \rho_g \times V_a \times C_{\text{STP}} = \frac{\varphi \times (1 - S_w - S_o) \times \rho_g \times C_{\text{STP}}}{\rho_{\text{bulk}}} - V_0 \exp \left\{ -D \left[\ln \left(\frac{\rho_a}{\rho_g} \right) \right]^k \right\} \times \frac{\rho_g}{\rho_a} \quad (18)$$

$$\begin{aligned} \text{GIP} &= n_{\text{abs}} + n_f \\ &= V_0 \exp \left\{ -D \left[\ln \left(\frac{\rho_a}{\rho_g} \right) \right]^k \right\} + \frac{\varphi \times (1 - S_w - S_o) \times \rho_g \times C_{\text{STP}}}{\rho_{\text{bulk}}} \\ &\quad - V_0 \exp \left\{ -D \left[\ln \left(\frac{\rho_a}{\rho_g} \right) \right]^k \right\} \times \frac{\rho_g}{\rho_a} \\ &= V_0 \exp \left\{ -D \left[\ln \left(\frac{\rho_a}{\rho_g} \right) \right]^k \right\} \times \left(1 - \frac{\rho_g}{\rho_a} \right) \\ &\quad + \frac{\varphi \times (1 - S_w - S_o) \times \rho_g \times C_{\text{STP}}}{\rho_{\text{bulk}}} \end{aligned} \quad (19)$$

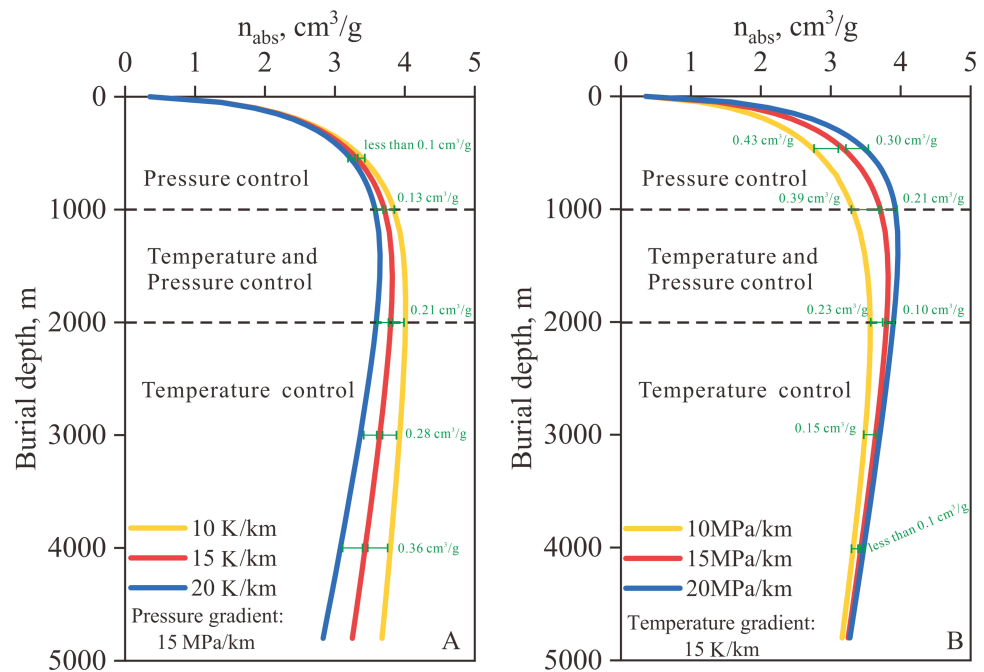
where n_f^{con} (cm³/g) is the free gas amount calculated without subtracting the adsorption space volume, φ (%) is the rock porosity, S_w (%) is the reservoir water saturation, S_o (%) is the reservoir oil saturation, C_{STP} is the parameter for converting 1 g methane to 1 cm³ methane under standard conditions, with a value of 1400, ρ_{bulk} (g/cm³) is the bulk density of the rock, and n_f (cm³/g) is the actual free gas amount.

5.3.2 Influence of temperature and pressure

Based on the HPMA experiment and Eq. (13), n_{abs} increases with rising pressure and decreases with increasing temperature. However, as the burial depth of the shale reservoir increases, both temperature and pressure rise simultaneously. Thus, it is challenging to directly determine whether n_{abs} increases or decreases with increasing burial depth. Different temperature gradients (10 K/km, 15 K/km, 20 K/km) and pressure gradients (10 MPa/km, 15 MPa/km, 20 MPa/km) were respectively set. Assuming that the surface temperature and pressure in the study area are 288.15 K and 0.101 MPa, respectively, taking the DY1H-3 sample as an example, the longitudinal variations of n_{abs} under different temperature and pressure gradients were calculated (see Fig. 8).

High temperature inhibits the presence of adsorbed gas in shale. Under the same burial depth, the larger the temperature gradient, the smaller the n_{abs} (Fig. 8A). In shallow layers within 500 m, the variation in n_{abs} among different temperature gradients is minimal, less than 0.1 cm³/g. As the burial depth increases, the difference in n_{abs} values under different temperature gradients gradually widens. At depths of 1000 m, 2000 m, 3000 m, and 4000 m, the differences in n_{abs} among different temperature gradients are 0.13 cm³/g, 0.21 cm³/g, 0.28 cm³/g, and 0.36 cm³/g, respectively.

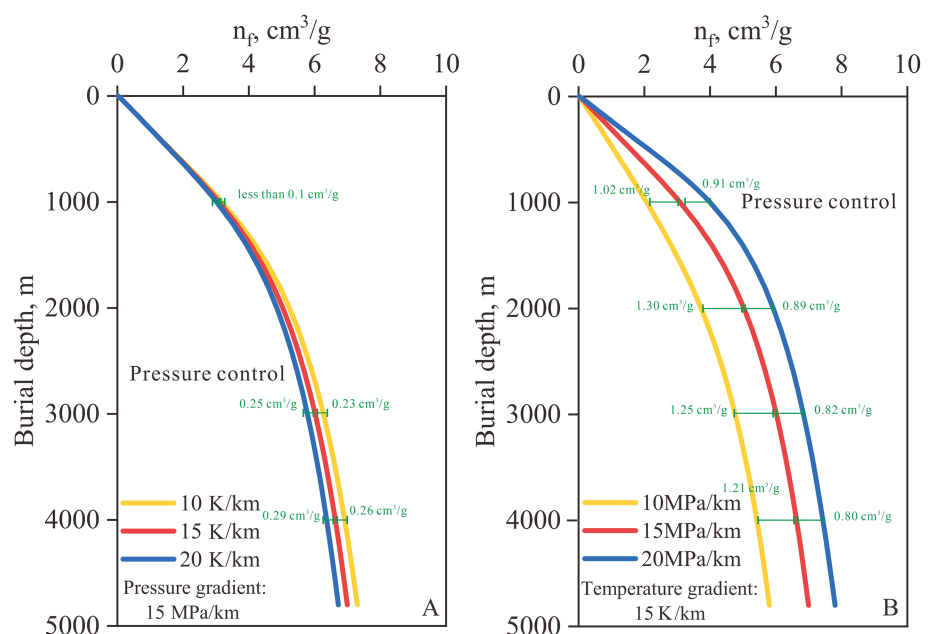
Fig. 8 Variation of longitudinal n_{abs} under different temperature (A) and pressure (B) gradients



High pressure promotes the presence of adsorbed gas in shale. Under the same burial depth, the larger the pressure gradient, the greater the n_{abs} (Fig. 8B). In shallow layers around 500 m, the difference in n_{abs} among different pressure gradients reaches its maximum. The differences in n_{abs} between the 15-MPa/km pressure gradient and the 10-MPa/km and 20-MPa/km gradients are 0.43 cm^3/g and 0.30 cm^3/g , respectively. Subsequently, as the burial depth increases, the difference in n_{abs} gradually starts to decline.

It is concluded that the main controlling factors of adsorbed gas content vary with different burial depths. In shallow regions where the burial depth is less than 1000 m, reservoir pressure predominantly controls the adsorbed gas content, and n_{abs} increases with rising pressure. At intermediate burial depths between 1000 and 2000 m, both reservoir pressure and temperature equally influence the adsorbed gas content. Under the combined effect of pressure and temperature, n_{abs} increases gradually and reaches its maximum around 2000 m. In deep areas with a burial

Fig. 9 Variation of longitudinal n_f under different temperature (A) and pressure (B) gradients



depth greater than 3000 m, reservoir temperature becomes the dominant controlling factor for adsorbed gas content, and n_{abs} decreases as temperature rises. The burial depth of P_3w^3 in Well DY1H ranges from 4328 to 4348 m. The *in-situ* adsorbed gas content is more significantly affected by reservoir temperature, and it decreases with increasing burial depth.

Similarly, to investigate the effects of temperature and pressure on free gas content, we analyzed sample DY1H-3, which has a porosity of 6.22% and rock density of 2.39 g/cm³. Since liquid oil cracked during high-maturity thermal evolution, oil saturation (S_o) is 0. By neglecting formation water saturation effects ($S_w = 0$) on n_f , we calculated longitudinal n_f distributions under different temperature and pressure gradients (Fig. 9).

The results indicate that, at the same burial depth, the larger the temperature gradient, the smaller the n_f ; conversely, the greater the pressure gradient, the larger the n_f . Notably, at a given depth, the differences in n_f between different pressure gradients are substantially larger than those among different temperature gradients (Fig. 9), which reveals that reservoir pressure is the primary factor governing the free gas content in both shallow and deep burial zones, while the influence of reservoir temperature is relatively weak. Consequently, the *in-situ* free gas content of P_3w^3 is more significantly affected by reservoir pressure, and it gradually increases with the burial depth.

To more intuitively demonstrate the contribution of adsorbed and free gas to the GIP in the vertical direction, the longitudinal proportion variation diagrams of n_{abs} and n_f under different temperature and pressure gradients were made (Fig. 10A, B). Under different temperature gradients, there was no obvious proportion change, but, under different

pressure gradients, it could be clearly observed that, with the increase of pressure gradient, the proportion of deep n_f increased significantly. The longitudinal variation diagram of GIP also showed that, with the increase of burial depth (Fig. 10C), GIP continuously increased, indicating that for deep shale reservoirs, the promoting effect of pressure on n_f was greater than the inhibitory effect of temperature on n_{abs} , so that, with the increase of burial depth, GIP continuously increased and the proportion of n_f continuously increased.

5.3.3 *In-situ* gas content

Actual stratigraphic reservoirs contain formation moisture, which is widely recognized to significantly reduce methane adsorption capacity. Studies conducting high-pressure methane adsorption experiments on moisture-equilibrated shale have demonstrated that V_0 values under wet conditions typically range from 20% to 80% of dry-condition values, averaging 64.9% (Gasparik et al. 2014; Merkel et al. 2016; Shabani et al. 2018). This proportional factor has therefore been applied in this paper to adjust methane adsorption capacity estimates for water-bearing shale reservoirs. The P_3w^3 shale samples exhibited average TOC content of 7.68% and average porosity of 6.05%. Geological data from Well DY1H indicate formation temperature and pressure gradients of 10 K/km and 20 MPa/km, respectively. With water saturation (S_w) at 15%, the average adsorbed gas content, free gas content, and *in-situ* gas content of the actual P_3w^3 shale reservoir are calculated to be 2.47 cm³/g, 6.19 cm³/g and 8.66 cm³/g, respectively (the ratio of free gas to adsorbed gas is 7:3). These values are significantly higher than those of the Wufeng–Longmaxi shale under the same geological

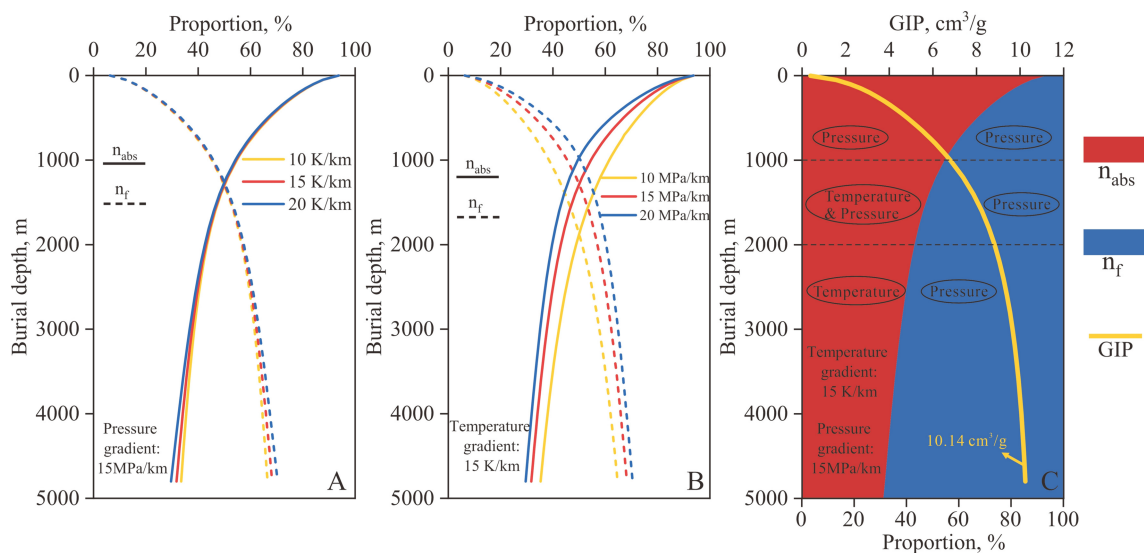
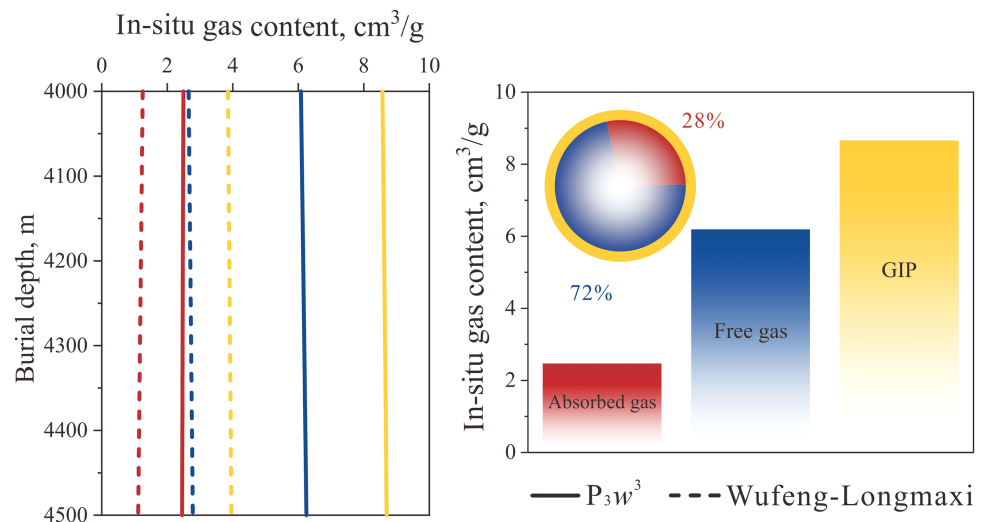


Fig. 10 Proportion of longitudinal n_{abs} and n_f under different temperature (A) and pressure (B) gradients and variation of longitudinal GIP (C)

Fig. 11 Adsorbed gas, free gas, and GIP in P_3w^3 shale and compared with Wufeng–Longmaxi shale



conditions (1.18 cm³/g, 2.75 cm³/g, and 3.93 cm³/g, respectively) (Fig. 11; Zhang et al. 2023b).

5.4 Research limitations and future direction

Although this study clarifies the adsorption mechanism of the P_3w shale, identifies the determinants controlling its high gas content, and restores its *in-situ* gas content, these findings provide critical insights into shale gas resource evaluation and development strategies in the eastern Sichuan Basin. However, there are still some limitations.

Firstly, actual shale reservoirs exist under formation moisture equilibrium conditions, where adsorption capacity is typically lower than that measured in our dried laboratory samples. Although we adjusted the V_0 values in the S-DA model based on proportional factor of previous studies, deviations from the actual reservoir in the study area may persist. To address this, future work will involve conducting high-pressure methane adsorption experiments on different moisture content shale samples to accurately evaluate the true adsorption capacity of the P_3w shale.

Secondly, conducting adsorption measurements directly on shale samples cannot distinguish the individual contributions of different components. Therefore, in future work, we will perform high-pressure methane adsorption tests on separated kerogen and clay mineral fractions extracted from P_3w shale samples. This approach will quantify adsorption contributions of shale organic and inorganic components separately.

6 Conclusions

1. The S-DA model exhibits the best fitting performance when restoring the excess adsorption amount to the absolute adsorption amount for P_3w shale in the eastern

Sichuan Basin. Methane is preferentially adsorbed by P_3w shale micropores with high adsorption potential. Once micropore-filling is nearly saturated, monolayer adsorption forms on the meso-/macropore surface.

2. The P_3w shale in eastern Sichuan Basin was deposited in a deep-water shelf environment under anoxic and reducing conditions, where well-preserved biological remains provided the material basis for organic matter enrichment. The high TOC content of the P_3w^3 shale was the main controlling factor for its high adsorbed gas content. Furthermore, the anti-compaction and pore-preservation effects of siliceous minerals mitigated porosity reduction during diagenesis. The high porosity of P_3w^3 shale was the main controlling factor for its high free gas content. Consequently, the 10- to 15-m-thick siliceous shale interval exhibiting both high TOC content and elevated porosity in the P_3w^3 represents the strategic exploration target.
3. The *in-situ* adsorbed gas content of P_3w shale in the eastern Sichuan Basin decreases with rising reservoir temperature, while the *in-situ* free gas content increases with rising reservoir pressure. Under the combined effect of temperature and pressure, the *in-situ* gas content increases as the burial depth increases. For the P_3w^3 shale with a burial depth of 4300–4400 m, the shale gas reservoir is mainly in the free state, and the ratio of free gas to adsorbed gas is approximately 7:3. Therefore, development should employ high-intensity fracturing to improve reservoir permeability for free gas production, complemented by CO₂ injection to enhance methane desorption through competitive adsorption mechanisms. This will achieve the efficient exploitation of the P_3w shale.

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Declarations

Conflict of interest The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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